High-accuracy measurements of total column water vapor from the Orbiting Carbon Observatory-2

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Key Points:

· OCO-2 can measure total column water vapor with high precision, accuracy, and spatial resolution over land and ocean surfaces

· OCO-2 is the first space-based sensor to simultaneously measure the two most important greenhouse gases, water vapor and carbon dioxide

· OCO-2 water vapor measurements may be useful in improving numerical weather predictions and acting as a validation source for other sensors

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Abstract

Accurate knowledge of the distribution of water vapor in Earth's atmosphere is of critical importance to both weather and climate studies. Here we report on measurements of total column water vapor (TCWV) from hyperspectral observations of near-infrared reflected sunlight over land and ocean surfaces from the Orbiting Carbon Observatory-2 (OCO-2). These measurements are an ancillary product of the retrieval algorithm used to measure atmospheric carbon dioxide concentrations, with information coming from three highly resolved spectral bands. Comparisons to high-accuracy validation data, including ground-based GPS and microwave radiometer data, demonstrate that OCO-2 TCWV measurements have maximum root mean square deviations of 0.9-1.3 mm. Our results indicate that OCO-2 is the first space-based sensor to accurately and precisely measure the two most important greenhouse gases, water vapor and carbon dioxide, at high spatial resolution (1.3×2.3 km^2), and that OCO-2 TCWV measurements may be useful in improving numerical weather predictions and reanalysis products.

1 Introduction

The Orbiting Carbon Observatory-2 (OCO-2) [*Crisp et al.*, 2008] was launched on 2 July 2014 with the goal of using hyperspectral observations of near-infrared reflected sunlight to measure the column-averaged dry-air mole fraction of carbon dioxide (X_{CO_2}) with the accuracy and precision needed to constrain net carbon dioxide (CO_2) fluxes on regional scales. While CO_2 sources and sinks currently represent a large scientific uncertainty, knowledge of water (H_2O) is also critical in understanding our planet. Water vapor, specifically, is important in how it influences the radiation budget, hydrologic cycle, weather patterns, and climate change. Improved knowledge of water vapor could lead to an enhanced understanding in all of these fields.

Currently, global spaced-based information on water vapor comes from a number of satellite instruments. First, there are sensors that operate at microwave wavelengths such as the Special Sensor Microwave Imager [*Wentz and Spencer*, 1998], the Advanced Microwave Scanning Radiometer Earth Observing System, the Advanced Microwave Scanning Radiometer-2 (AMSR-2), the Tropical Rainfall Measuring Mission Microwave Imager, and the Global Precipitation Measurement Microwave Imager. Second, sensors that operate at thermal infrared wavelengths such as the Atmospheric Infrared Sounder (AIRS; *Susskind et al.* [2003]), the Infrared Atmospheric Sounding Interferometer (IASI; *Pougatchev*

et al. [2009]), the Cross-track Infrared Sounder [*Bloom*, 2001], and the High-resolution Infrared Radiation Sounder [*Bates and Jackson*, 2001]. Finally, sensors that operate at near-infrared wavelengths such as the Moderate Resolution Imaging Spectroradiometer (MODIS) [*Gao and Kaufman*, 2003; *Albert et al.*, 2005] and the MEdium Resolution Imaging Spectrometer (MERIS) [*Bennartz and Fischer*, 2001; *Lindstrot et al.*, 2012]. Over ocean, microwave and infrared sensors are typically used, as the surface temperature and emissivity are relatively well-known. Over land, emissivity constraints result in a preference towards near-infrared sensors. However, all of these sensors have limitations in terms of accuracy, spatial resolution, and spatial coverage.

OCO-2 measures reflected sunlight in clear-sky scenes over both land and ocean and is at the front of NASA's Afternoon Constellation [*L'Ecuyer and Jiang*, 2010]. It is a clear-sky instrument because of the large errors typically induced by severe light path modification effects caused by scenes containing an appreciable amount of clouds or aerosols. It makes eight measurements simultaneously across a narrow (<10 km) swath every 2.3 km. This orbital path and subsequent co-location with other satellites makes OCO-2 well-suited to provide robust and well-calibrated products over much of the globe. OCO-2 uses high-resolution grating spectrometers with a resolving power greater than 18,000 to measure light in three spectral bands centered at approximately 0.76, 1.61, and 2.06 μm. The primary OCO-2 X_{CO_2} retrieval algorithm is referred to as the ACOS (Atmospheric Carbon Observations from Space; *O'Dell et al.* [2012, 2016]) algorithm, and uses optimal estimation [*Rodgers*, 2000] to estimate X_{CO_2} and a number of other quantities that impact the X_{CO_2} retrieval. These additional quantities include aerosol optical depth and height, surface pressure, and surface albedo. At the near-infrared wavelengths that OCO-2 observes, there are many H_2O lines present. If these absorption features and their broadening impact on the CO_2 lines are not accounted for, biases are introduced into the X_{CO_2} retrieval. Thus, one of the retrieved variables in the ACOS algorithm is total column water vapor (TCWV), which is defined as the total gaseous water contained in a vertical column of atmosphere. The unit of TCWV throughout this work is the millimeter (mm), where 1 mm is equal to 1 kg/m^2. Absorption coefficient tables (ABSCO v4.2; *Gordon* [2012]) are used to supply absorption cross section values for the retrieved gases and are critically important in retrieving nearly bias-free measurements. The inclusion of TCWV in the ACOS retrieval leads to the following question: how well can OCO-2 retrieve H_2O information?

In this work, we evaluate the precision and accuracy of OCO-2 TCWV measurements via simulations and comparisons to multiple independent validation sources. We then discuss improvements that could be made to the retrieval algorithm as well as potential applications of the water vapor product.

2 Theoretical Basis

As water is a non-linear molecule with a net dipole moment, many rotational and vibrational absorption features exist throughout the electromagnetic spectrum. OCO-2 resolves a number of strong H_2O absorption features in both its 1.61 and 2.06 μm bands. Figure 1 shows an example of absorption features in these bands, as seen through the OCO-2 spectral response function. While the majority of the lines are due to carbon dioxide, many water vapor lines are also evident. In an atmosphere devoid of clouds and aerosols, the relative line depth is directly related to TCWV. The lines are well-resolved, and because of OCO-2's high signal-to-noise ratio of several hundred to greater than 1000 [*Frankenberg et al.*, 2015; *Eldering et al.*, 2016], even small changes in the relative line depth can be detected.

The ACOS algorithm uses the European Centre for Medium-Range Weather Forecasts Integrated Forecast System (ECMWF IFS; *ECMWF* [2015]) for meteorological a priori information on temperature, water vapor, and surface pressure and retrieves a single scaling factor applied to the ECMWF water vapor profile. This is done to reduce possible correlations between the retrieved X_{CO_2} and water vapor. Because the ACOS algorithm is given the precise spectral response function and SNR of the instrument, the optimal estimation approach produces an estimate of the uncertainty in its retrieved TCWV. This estimate is typically only 0.1-0.2 mm and includes errors due to both instrument noise as well as cross-talk errors due to other retrieved variables such as aerosols and carbon dioxide. However, the estimate does not include errors in the prescribed ECMWF vertical profile of water vapor and may not fully account for errors due to clouds and aerosols, so it may be an underestimate. This theoretical uncertainty therefore serves as a useful lower limit of the actual TCWV retrieval error.

We next improve on this estimate by performing retrievals on simulated spectra in realistic atmospheres. These atmospheres were created using the Colorado State University (CSU) Orbit Simulator (see *O'Brien et al.* [2009] for details), and include realistic

representations of the viewing geometry and surface reflectance, profiles of clouds and aerosols from the Cloud–Aerosol Lidar with Orthogonal Polarization (CALIOP) instrument onboard the Cloud–Aerosol Lidar and Infrared Pathfinder Satellite Observations (CALIPSO; *Winker et al.* [2009]), and meteorology from ECMWF. Gaussian instrument noise is also added to the spectra. For more details on the methodology, see *O'Dell et al.* [2012]. Scenes contaminated by clouds and aerosols are rejected via a spectral-based cloud-screening technique [*Taylor et al.*, 2012, 2016], as OCO-2 is only able to make accurate retrievals in scenes nearly free of cloud and aerosol contamination. However, scenes passing this pre-filter may still contain some clouds and aerosols, typically with an optical depth less than 0.3.

ACOS retrievals were then performed on scenes passing the cloud and aerosol pre-filter. To challenge our retrieval, we set the prior meteorological data to be from the National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR) Reanalysis-1 [*Kalnay et al.*, 1996], rather than from ECMWF, as a proxy for realistic errors in water vapor amount and vertical distribution, as well as errors in the temperature profile and surface pressure. Despite these errors sources, we were able to retrieve TCWV values with an almost perfect correlation with the true water vapor (R=0.999) and effectively no bias (-0.08 mm) compared to the true TCWV used to create the synthetic measurements (see Figure S1 in the supplementary material). The root mean squared deviation (RMSD) between the retrieved TCWV and true TCWV was reduced from about 4 mm (7 mm) in the prior to 0.39 mm (0.75 mm) in the retrieval over land (ocean) (see Tables S1 and S2 in the supplementary material). This mean error of about 0.6 mm is higher than the simple theoretical estimate of approximately 0.1-0.2 mm likely because of additional cloud and aerosol light-path modification effects but also potentially because of errors in the prior temperature profile, surface pressure, and water vapor profile shape.

3 Data Description

We now extend our analysis to real OCO-2 data by comparing OCO-2 TCWV measurements to four TCWV validation sources: SuomiNet [*Ware et al.*, 2000], the AErosol RObotic NETwork (AERONET) [*Holben et al.*, 1998], the Integrated Global Radiosonde Archive (IGRA) [*Durre et al.*, 2006], and the Advanced Microwave Scanning Radiometer-2 (AMSR-2) [*Imaoka et al.*, 2010]. SuomiNet is a ground-based Global Positioning Sys-

tem (GPS) network that measures TCWV concentrations using the time delay in the 1.6 and 1.2 GHz GPS signals. As a GPS satellite passes overhead, the transmitted signal is slowed by Earth's atmosphere and the time it takes to reach a given SuomiNet instrument on the ground is recorded. The delay in this time is a function of how much water vapor is in the column of air, the temperature profile, etc. Using a simple equation, TCWV can then be retrieved with an estimated accuracy of 1-2 mm [*Ware et al.*, 2000]. AERONET is a ground-based sun-photometer network primarily designed to measure aerosol properties. Each AERONET instrument tracks the sun as it travels across the sky and uses measured radiances to infer column values of several quantities, including water vapor (using a band around 0.94 μm via the Direct Sun Algorithm version 2) [*Reagan et al.*, 1987; *Schmid et al.*, 1996] with a reported accuracy of better than 2 mm [*Michalsky et al.*, 1995]. IGRA is a collection of radiosonde and pilot balloon observations from over 1,500 globally distributed stations. While primarily used for operational weather forecasting, radiosonde observations have also been used for other applications including the verification of satellite measurements. *Yu et al.* [2015] found mean differences in TCWV between radiosondes and a ground-based microwave radiometer of 0.9 mm. An exponential fit to each IGRA profile was used to account for any water vapor present above the altitude at which the radiosonde stopped taking data. Only Vaisala RS92s were used in this study, as they have been extensively validated (e.g. *Yu et al.* [2015]; *Wang et al.* [2013]). We also required each profile to contain at least 30 vertical measurements. The primary limitation of these three ground-based networks is their lack of coverage over ocean and sparse coverage over land, which restricted the number of co-locations as OCO-2's orbit track is less than 10 km wide and has a repeat cycle of approximately 16 days. Additionally, the infrequent launch times of radiosondes (typically only 0Z and 12Z) further restrict the number of available co-locations of IGRA with OCO-2. The fourth validation source, AMSR-2, is a radiometer that measures water vapor at microwave wavelengths over ocean using horizontally and vertically polarized channels at 18.7, 23.8, and 36.5 GHz. It flies in the Afternoon Constellation a few minutes behind OCO-2 and thus provides a substantial number of co-located measurements. *Duncan and Kummerow* [2016] found a RMSD between AMSR-2 and a radiosonde dataset of 2.6 mm. For this work, the Remote Sensing Systems 0.25° gridded TCWV product was used (version 7.2; *Wentz et al.* [2014]). The MODIS instrument on NASA's Aqua satellite, despite being in the Afternoon Constellation with OCO-2, was not selected as a validation source, as its water vapor errors are likely larger

than those from OCO-2 (e.g. *Gao and Kaufman* [2003]; *Li et al.* [2003]; *Diedrich et al.* [2015]).

To compare to OCO-2 TCWV measurements to SuomiNet and AERONET, co-location criteria of 30 minutes in time and 0.1° latitude (about 11 km) in space were chosen. We examined the potential of expanding the co-location thresholds in order to increase the number of matched measurements but found that the differences between the OCO-2 and validation TCWV values increased substantially for larger thresholds, indicating that the spatial and temporal variability of water vapor imposes limits on the chosen co-location thresholds. Supplementary Figure S2 shows a minimum in RMSD between OCO-2 and SuomiNet TCWV using a co-location distance threshold of about 0.1° latitude. Smaller spatial co-location thresholds than about 0.1° have a larger RMSD because there are too few remaining SuomiNet measurements. In an attempt to increase the number of IGRA co-locations, we allowed radiosondes within 0.1° to have been launched up to an hour before the corresponding OCO-2 measurement, as radiosonde balloons typically take 1-2 hours to ascend through the atmosphere. We also applied a station surface pressure or station altitude difference threshold to ensure that OCO-2 wasn't measuring substantially shorter or longer path lengths (and thus retrieving less or more water vapor, which is concentrated near the surface). Against SuomiNet and IGRA, a surface pressure difference threshold of less than 10 hPa was used while against AERONET an altitude difference threshold of less than 100 m was used. The chosen thresholds removed expected biases that were appearing when OCO-2 measurements were sampling columns of air much higher or lower in elevation than the nearby SuomiNet, AERONET, or IGRA station. We chose to reject data instead of trying to apply a custom water vapor correction because water vapor is highly concentrated near the surface and thus any errors or uncertainty in the correction could represent a disproportionately large fraction of the total TCWV.

OCO-2 measurements (ACOS B7 lite files) [*Eldering et al.*, 2016] from 6 September 2014 to 10 February 2016 were used for this study. This represents a majority of the currently available OCO-2 measurements, as the satellite was launched in the summer of 2014. As was done for the simulated measurements, the pre-filter of *Taylor et al.* [2012, 2016] was used to eliminate scenes contaminated by clouds and aerosols. Despite this, some poor retrievals remain in the dataset, typically due to uncorrected cloud and aerosol effects. The ACOS B7 "lite" files used at the time of this writing only include data pass-

ing an additional "warn-level" based filter (warn level less than 17, see *Mandrake et al.* [2013, 2015] for details).

OCO-2 nadir and glint measurements over land and glint measurements over ocean were used for this study. Glint geometry, where the satellite views a surface footprint near the sun-glint spot on the earth's surface, is primarily used over oceans but, due to satellite maneuvering restrictions, is also used over land. Land has a sufficiently strong surface reflectance in glint geometry and thus enables the use of glint measurements along with nadir (downward looking) measurements. Target mode measurements, where OCO-2 dithers across a specific target and gathers thousands of measurements, were excluded from the main analysis. This was to avoid having the statistics overly influenced by a large number of measurements co-located with a small number of validation measurements. The target mode measurements, however, agreed with our overall conclusions (see Table S3 in supplementary material). Figure 2 shows the location of the 282 SuomiNet stations, 83 AERONET stations, 12 IGRA stations, and 229,390 0.25°x0.25° AMSR-2 grid cells that had at least one co-located OCO-2 measurement for this study.

As previously stated, OCO-2 uses ECMWF model output as its meteorological prior. This gave us an opportunity to see if the OCO-2 retrieval is able to improve upon model output, which would indicate that OCO-2 TCWV measurements may be useful in improving numerical prediction models. Additionally, we co-located OCO-2 TCWV measurements with a reanalysis data product, the Modern-Era Retrospective analysis for Research and Applications (Version 2 of MERRA-2; *Bosilovich et al.* [2015]), to provide a model comparison independent of the OCO-2 retrieval framework.

4 Validation

Comparing OCO-2 TCWV measurements to our four validation sources, Figure 3 demonstrates that ACOS is able to retrieve TCWV with relatively high accuracy and small biases. The ECMWF TCWV values, used as the prior, have RMSDs of about 2.2 mm, 3.4 mm, 2.6 mm, and 2.3 mm relative to SuomiNet, AERONET, IGRA, and AMSR-2, respectively (see Figure S3 and Table S4 in the supplementary material). The OCO-2 retrievals (Figure 3) are able to reduce these RMSDs down to about 1.3 mm, 2.1 mm, 1.8 mm, and 0.9 mm. The correlation coefficients relative to the prior are improved against all four validation sources and represent a reduction in error variance of 65%, 69%, 55%, and

87% for SuomiNet, AERONET, IGRA, and AMSR-2, respectively. The mean bias relative to SuomiNet, IGRA, and AMSR-2 are 0.3, 0.4 mm, and -0.4 mm, respectively, while the AERONET TCWV measurements appear to be low biased by approximately 1.4 mm (see Table S3 in the supplementary material). The slope of the best-fit line for AERONET is about 1.08 which equates to a low bias of 8% relative to the retrieved OCO-2 TCWV values. In addition to ECMWF, MERRA-2 was also found to have worse error statistics than OCO-2, relative to the validation sources. We found RMSDs of 2.8 mm, 3.4 mm, 3.3 mm, and 2.8 mm relative to SuomiNet, AERONET, IGRA, and AMSR-2, respectively (see Figure S4 and Table S5 in the supplementary material). A summary of the RMSDs between MERRA-2, ECMWF, and OCO-2 and the four validation sources is shown in Figure 4.

Regional biases were difficult to examine for SuomiNet, AERONET, and IGRA due to their limited global coverage. The comparison of OCO-2 to AMSR-2, however, showed small latitudinal biases (<5%) in TCWV, with AMSR-2 having larger TCWV values, especially in the tropics and far southern latitudes (see supplementary Figure S5). Additional study is needed to identify the source of these differences.

Finally, our results were not significantly dependent on the observation mode (nadir, glint, target) of OCO-2 nor were they dependent on the quality flag (a binary flag derived from several metrics, which indicates the overall quality of the final X_{CO_2} product) or warn level. For example, the RMSD between OCO-2 and SuomiNet TCWV for all quality flags is 1.38 ppm, compared to 1.34 ppm for only "good" quality flags. This indicates that potentially many more OCO-2 measurements with "low quality" X_{CO_2} values may still have a TCWV measurement with comparably small errors. This is partly because the precision requirements for TCWV are less stringent than X_{CO_2}, i.e. about 1 part in 10-60 (1 mm precision for a typical range of TCWV values) vs. 1 part in 200 for X_{CO_2} (2 ppm precision for typical X_{CO_2} values).

5 Discussion

Our initial analysis of retrievals performed on synthetic measurements demonstrated that ACOS can accurately retrieve TCWV in simulated conditions and that improvement over the prior in real retrievals is to be expected. The comparison of OCO-2 TCWV measurements to four independent validation sources revealed that OCO-2 is able to accurately and precisely measure TCWV. Small biases and standard deviations were found when

OCO-2 TCWV was compared to SuomiNet, IGRA, and AMSR-2, while it was found that AERONET may have a mean low bias of approximately 1.4 mm (8%). This is approximately in agreement with the 5-6% low bias in AERONET found by *Pérez-Ramírez et al.* [2014]. The small biases between OCO-2 and SuomiNet (+0.34 mm), IGRA (+0.41 mm) and AMSR-2 (-0.44 mm) may partly be a result of biases in SuomiNet, IGRA and AMSR-2 themselves, as absolute water vapor calibration is difficult to achieve. However, these bias and scatter estimates, comprised of errors in OCO-2, the validation sources, and co-location errors, still provide a useful upper limit on the true OCO-2 TCWV errors. Using the most accurate validation source over land (SuomiNet) and our sole validation source over ocean (AMSR-2) leads to a TCWV RMSD upper limit of 0.9-1.3 mm. This error range is larger than that predicted by our simulated tests. Potential sources of these extra errors include imperfect spectroscopy, aerosol and cloud contamination, other forward model errors, and co-location errors. The comparison of OCO-2 to the four validation sources suggests that the error statistics of the OCO-2 TCWV product are not substantially different over land and ocean. This is in contrast to other operational instruments that perform poorly over certain surface types. MERIS, for example, is sensitive to aerosols and their distribution over ocean surfaces, which can result in large errors (≥ 5 mm, *Lindstrot et al.* [2012]). OCO-2, however, uses its glint mode over ocean, resulting in high signal-to-noise ratios and thus less sensitivity to aerosol layers.

As this study was done with the operational ACOS algorithm, which was designed for CO_2 and only contained H_2O as an ancillary product, improvements specifically related to water vapor might enable even more accurate H_2O retrievals from OCO-2. Upgrades to the water vapor spectroscopy, improved aerosol parameterizations, and more elaborate water vapor retrieval schemes could all result in more information about water vapor being extracted from the measured radiances. For example, above-cloud retrievals of water vapor are likely possible with OCO-2, which would vastly increase the number of valid measurements (as cloudy scenes are currently screened out). This analysis, however, is beyond the scope of this study.

Our results give evidence that OCO-2 may be accurate enough to be used as a validation source for reanalysis products as well as other methods of measuring TCWV (e.g. MODIS, MERIS, the Suomi National Polar-orbiting Partnership (NPP), AIRS, IASI). Additionally, OCO-2 coverage, while limited by its narrow yet dense ground-track, covers both land and ocean over much of the low- and mid-latitudes. This means these TCWV

measurements may be useful in improving numerical weather prediction models, which are dependent on the assimilation of accurate water vapor measurements. However, further work must be done to determine if measurements from OCO-2 can provide water vapor information not already measured by other instruments. Besides showing how OCO-2 is able to improve upon the ECMWF prior, we also briefly compared the MERRA-2 reanalysis product to our validation sources and found that OCO-2 would be able to improve upon MERRA-2 as well. These model RMSDs, visualized in Figure 4, are considerably larger than the RMSDs between OCO-2 and the validation sources, which provides additional evidence that OCO-2 TCWV measurements may be useful for numerical weather prediction and data assimilation applications over land and ocean.

6 Conclusions

In this work we validate measurements of total column water vapor from hyperspectral, near-infrared measurements of reflected sunlight made by OCO-2 over both land and ocean. We find that theoretical single-sounding TCWV errors are approximately 0.6 mm while comparisons to validation sources reveals that OCO-2 TCWV measurements are highly accurate, with RMSDs of 0.9-1.3 mm and mean biases typically of less than 0.5 mm. The results of this study show that OCO-2 is the first space-based instrument to accurately measure the most important natural greenhouse gas (water vapor) simultaneously with the most important anthropogenic greenhouse gas (carbon dioxide) [*Eldering et al.*, 2016], at high spatial resolution (1.3x2.3 km^2). These OCO-2 TCWV measurements may be useful regarding the improvement of numerical weather prediction models and reanalysis products along with acting as a validation source for other instruments. Additionally, future satellites with OCO-2-like capabilities, such as OCO-3, MicroCarb, GOSAT-2, and CarbonSat, may be able to measure water vapor with the same or better accuracy than OCO-2.

contained in the level-2 OCO-2 "Lite" files, available at the NASA Goddard Earth Sciences Data and Information Services Center (GES DISC, http://disc.sci.gsfc.nasa.gov/uui/datasets/OCO2_L2_Lite_FP_V7r/summary). The authors would like to thank Dr. Thomas H. Vonder Haar, Andrew I. Manaster, and Heather Q. Cronk for their contributions to this work.

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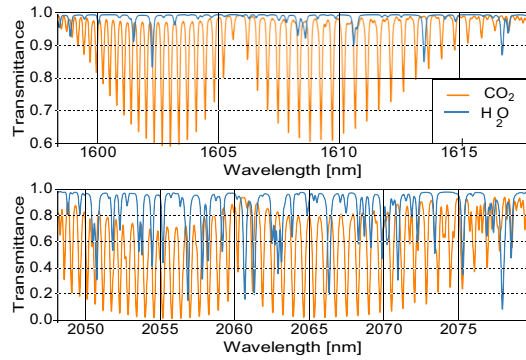
Figure 1. Simulated OCO-2 1.61 μm band (top panel) and 2.06 μm band (bottom panel) transmittance spectra in a typical downward-looking observation, demonstrating the prevalence of water vapor absorption features (blue) within the CO_2 absorption bands (orange).

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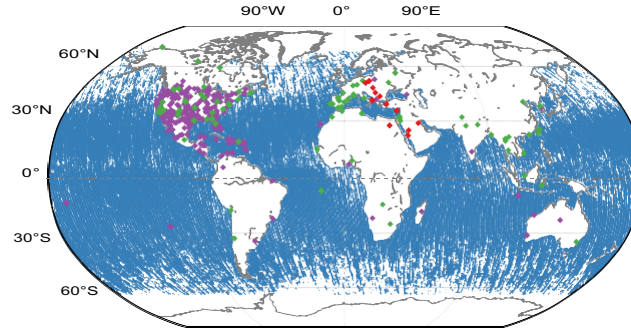
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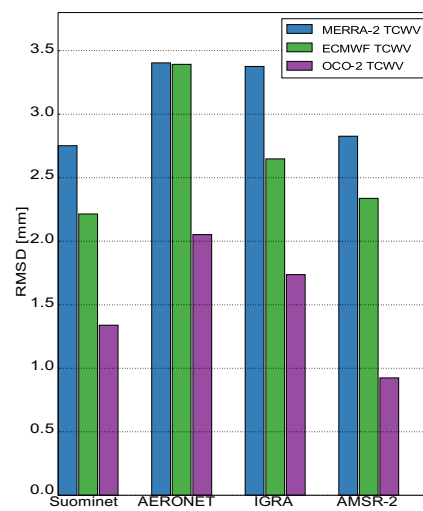
Figure 2. Location of SuomiNet sites (purple), AERONET sites (green), IGRA sites (red), and AMSR-2 grid cells (blue) that have a valid OCO-2 measurement co-located in time and space from 6 September 2014 to 10 February 2016.
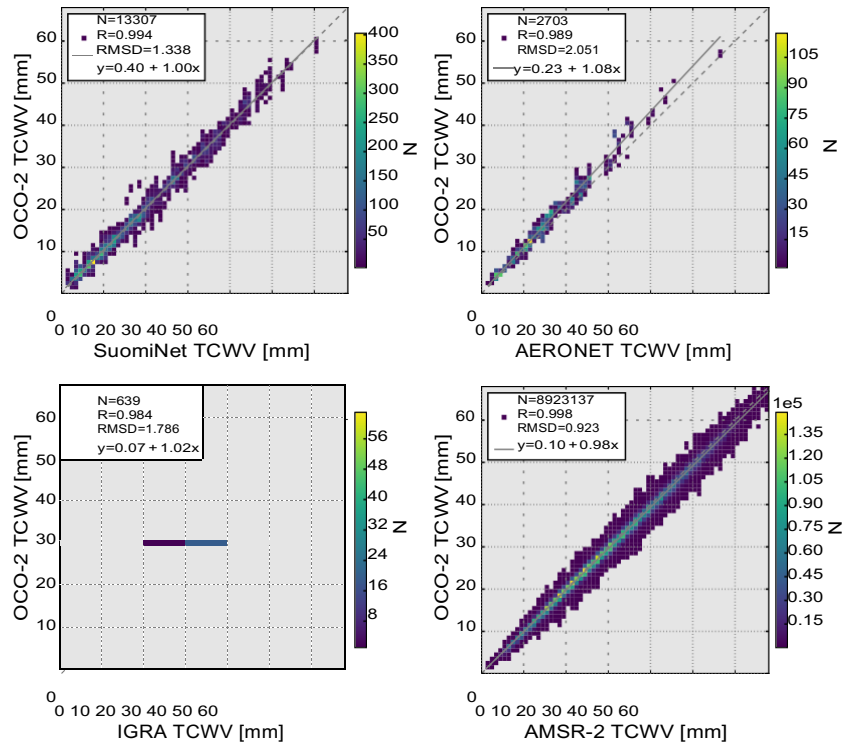
Figure 3. Heatmap comparison of the retrieved OCO-2 TCWV to SuomiNet, AERONET, IGRA, and AMSR-2 TCWV measurements.

456 **Figure 4.** RMSD between MERRA-2, ECMWF, and OCO-2 TCWV and all four validation sources

457 (SuomiNet, AERONET, IGRA, and AMSR-2).